AMENDMENTS TO THE CLAIMS

This listing of claims will replace all prior versions, and listings, of claims in the application.

Listing of Claims:

1-18. (cancelled).

19. (previously presented) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, wherein the chemical entities comprise a phosphate residue or a surrogate for a phosphate residue; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

b) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

c) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

20. (previously presented) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a CnA binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254 according to Figure 1, or a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, wherein the chemical entities comprise a phosphate residue or a surrogate for a phosphate residue;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

b) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

c) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

21. (currently amended) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314,

339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å, wherein the chemical entities comprise a hydrophobic core and a 10-14 Å linker, wherein the linker ~~that~~ projects a hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 115, 118 and 119 of CnB and amino acid residues 352, 353, 356 and 357 of CnA according to Figure 1, or amino acids of a CnA/CnB homologue that have a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part

of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b) docking said chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity wherein said docking utilizes energy minimization;

c) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

22. (currently amended) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a

binding pocket defined by CnA amino acids 90, 91, 92, 118, 120, 121, 122, 124, 150, 151, 156, 159, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 310, 311, 312, 313, 314, 317, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å, wherein the chemical entities comprise a hydrophobic core and a 10-14 Å linker, wherein the linker ~~that~~ projects a hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 115, 118 and 119 of CnB and amino acid residues 352, 353, 356 and 357 of CnA according to Figure 1, or amino acids of a CnA/CnB homologue that have a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

c) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associate with all or part of the CnA/CnB binding pocket or CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

23. (currently amended) A method for using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex defined by the entire set of structure coordinates of CnA/CnB amino acids according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å, wherein the chemical entities comprise a hydrophobic core and a 10-14 Å linker, wherein the linker ~~that~~ projects a hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 115, 118 and 119 of CnB and amino acid residues 352, 353, 356 and 357 of CnA according to Figure 1, or amino acids of a CnA/CnB homologue that have a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said molecule, molecular complex, or homologue thereof and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining all or part of said molecule, molecular complex,

or homologue thereof and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the molecule, molecular complex, or homologue thereof;

b) docking said chemical entity with all or part of the molecule, molecular complex, or homologue thereof by employing computational means which utilize said structure coordinates of all or part of the molecule, molecular complex, or homologue thereof or the chemical entity, wherein said docking utilizes energy minimization;

c) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the molecule, molecular complex, or homologue thereof;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associate with all or part of the molecule, molecular complex, or homologue thereof based on said quantified association of said chemical entity.

24. (previously presented) The method according to claim 23, wherein said molecular complex is defined by the structure coordinates of the amino acids of CnA, the

amino acids of CnB, FKBP12 and FK506 according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å.

25. (previously presented) The method according to any one of claims 19-24, further comprising the steps of:

f) contacting the selected chemical entity with said molecule or molecular complex; and

g) monitoring the association of the molecule or molecular complex with the selected chemical entity.

26-30. (cancelled).

31. (previously presented) The method according to any one of claims 19, 20, 21 and 22, wherein prior to step a), further comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and

c) identifying all or part of said binding pocket.

32. (previously presented) The method according to claim 23, wherein prior to step a), further comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal.

33. (previously presented) The method according to any one of claims 19, 20, 21, 22 and 23 wherein the docking utilizes shape complementarity or is followed by molecular dynamics.

34. (previously presented) The method according to any one of claims 19, 20, 21, 22 and 23 wherein the docking is performed through visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of

said structure coordinates and structure coordinates of said chemical entity.

35. (previously presented) The method according to any one of claims 19-22, further comprising the steps of:

f) repeating steps a) to e) with a second set of a plurality of chemical entities that associate with all or another part of the binding pocket or homologue thereof;

g) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

h) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

36. (previously presented) The method according to claim 23 or 24, further comprising the steps of:

f) repeating steps a) to e) with a second set of a plurality of chemical entities that associate with all or another part of the molecule or molecular complex or homologue thereof;

g) optionally, visually inspecting the relationship of the selected first and second chemical entity to each other in relation to the molecule or molecular complex or homologue thereof on a computer screen using the three-dimensional graphical representation of the molecule or molecular complex or homologue thereof and said selected first and second chemical entity; and

h) assembling the selected first and second chemical entity into a compound or complex that associates with all or part of said molecule or molecular complex, or homologue thereof by model building.

37. (previously presented) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or

a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) identifying all or part of said binding pocket;

d) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

e) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue

binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

g) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

h) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

38. (previously presented) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254 according to Figure 1, or a CnA homologue binding

pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) identifying all or part of said binding pocket;

d) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

e) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which

utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

g) optionally repeating steps d) through f) with another of said plurality of chemical entities; and

h) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

39. (previously presented) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159,

161, and 162 according to Figure 1, or a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) identifying all or part of said binding pocket;

d) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

e) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

g) optionally repeating steps d) through f) with another of said plurality of chemical entities; and

h) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

40. (previously presented) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 124, 150,

151, 156, 159, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 310, 311, 312, 313, 314, 317, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said binding pocket and wherein said method comprises the steps of:

a) producing a crystal of a molecule or molecular complex comprising amino acids 5-168 of CnA and amino acids 24-370 of CnB and a chemical entity;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal;

c) identifying all or part of said binding pocket;

d) utilizing said structure coordinates defining all or part of said binding pocket and the structure coordinates of one of said plurality of chemical

entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

e) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

f) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

g) optionally repeating steps d) through f) with another of said plurality of chemical entities; and

h) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

41. (previously presented) The method according to any one of claims 37-40, further comprising the steps of:

i) contacting the selected chemical entity with said molecule or molecular complex; and

j) monitoring the association of the molecule or molecular complex with the selected chemical entity.

42. (previously presented) The method according to any one of claims 37-40, wherein the docking utilizes shape complementarity or is followed by molecular dynamics.

43. (previously presented) The method according to any one of claims 37-40, wherein the docking is performed through visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of said structure coordinates and structure coordinates of said chemical entity.

44. (previously presented) The method according to any one of claims 37-40, further comprising the steps of:

i) repeating steps d) to h) with a second set of a plurality of chemical entities that associate with all or another part of the binding pocket or homologue thereof;

j) optionally, visually inspecting the relationship of the selected first and second chemical entities to each other in relation to the binding pocket or homologue thereof on a computer screen using the three-dimensional graphical representation of the binding pocket or homologue thereof and said selected first and second chemical entity; and

k) assembling the first and second chemical entities into a compound or complex that associates with all or part of said binding pocket or homologue thereof by model building.

45. (currently amended) The method according to any one of claims 21-24, wherein the chemical entities further comprise a linker of 7-11 Å, wherein the linker ~~that~~ projects a second hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 341, 343, 344, and 352 of CnA and amino acid residue 123 of CnB according to Figure 1, or amino acids of a CnA/CnB homologue that have a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5 Å.

46. (previously presented) The method according to claim 45, wherein the second hydrophobic moiety comprises a hydrogen bond donor or acceptor that can form a hydrogen bond with all or any part of amino acid residues 341 and 352 of CnA according to Figure 1, or amino acids of a CnA homologue that have a root mean square deviation from the backbone atoms of said CnA amino acids of not more than 1.5 Å.

47. (currently amended) The method according to any one of claims 21-24, wherein the chemical entities further comprise a linker of 8-12 Å, wherein the linker ~~that~~ projects a second hydrophobic moiety from the center of the hydrophobic core to make a Van der Waals contact with all or part of amino acid residues 355 and 356 of CnA according to Figure 1, or amino acids of a CnA homologue that have a root mean square deviation from the backbone atoms of said CnA amino acids of not more than 1.5 Å.

48. (previously presented) The method according to claim 47, wherein the second hydrophobic moiety comprises a hydrogen bond donor or acceptor that can form a hydrogen bond with amino acid residue 359 of CnA according to Figure 1, or an amino acid of a CnA homologue that has a

root mean square deviation from the backbone atoms of said CnA amino acid of not more than 1.5 Å.

49. (previously presented) The method according to claim 24, wherein the hydrophobic core can make Van der Waals contact with all or part of amino acid residues 26, 46, 55, 56, 59 and 99 of FKBP12 according to Figure 1, or amino acids of a FKBP12 homologue that have a root mean square deviation from the backbone atoms of said FKBP12 amino acids of not more than 1.5 Å.

50. (previously presented) The method according to claim 49, wherein the hydrophobic core comprises a hydrogen bond donor or acceptor that can form a hydrogen bond with all or any part of FKBP12 amino acids 56 and 82 according to Figure 1, or amino acids of a FKBP12 homologue that have a root mean square deviation from the backbone atoms of said FKBP12 amino acids of not more than 1.5 Å.

51. (new) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of

CnA amino acids 122, 124, 125, 148, 150, 153, 155, 156, 160, 161, 220, 221, 222, 231, 232, 234, 235, 236, 237, 239, 253, 255, 256, 259, 282, 283, 284, 291, 302, 304, 313, 339, 340, 341, 342, 344, 345 and 346 according to Figure 1, or a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said CnA binding pocket and wherein said method comprises the steps of:

a) selecting a subset of CnA amino acid structure coordinates according to Figure 1, which are provided on a computer, to define all or part of said CnA binding pocket;

b) utilizing said structure coordinates defining all or part of said CnA binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

c) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue

binding pocket by employing computational means which utilize said structure coordinates of all or part of the CnA binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

d) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

52. (new) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A/calcineurin B (CnA/CnB) binding pocket defined by structure coordinates of CnA amino acids 341, 343, 344, 352, 353, 355, 356, 357, and 359 and CnB amino acids 115, 118, 119, and 123 according to Figure 1, or a CnA/CnB

homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said CnA/CnB binding pocket and wherein said method comprises the steps of:

a) selecting a subset of CnA/CnB amino acid structure coordinates according to Figure 1, which are provided on a computer, to define all or part of said CnA/CnB binding pocket;

b) utilizing said structure coordinates defining all or part of said CnA/CnB binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

c) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the CnA/CnB binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

d) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

53. (new) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said CnA binding pocket and wherein said method comprises the steps of:

a) selecting a subset of CnA amino acid structure coordinates according to Figure 1, which are provided on a computer, to define all or part of said CnA binding pocket;

b) utilizing said structure coordinates defining all or part of said CnA binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

c) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the CnA binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

d) analyzing the results of said docking to quantify the association between said chemical entity

and all or part of the CnA binding pocket or the CnA homologue binding pocket;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

54. (new) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254 according to Figure 1, or a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of

said CnA binding pocket and wherein said method comprises the steps of:

a) selecting a subset of CnA amino acid structure coordinates according to Figure 1, which are provided on a computer, to define all or part of said CnA binding pocket;

b) utilizing said structure coordinates defining all or part of said CnA binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA binding pocket or the CnA homologue binding pocket;

c) docking said chemical entity with all or part of the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the CnA binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

d) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA binding pocket or the CnA homologue binding pocket;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with all or part of the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

55. (new) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said CnA/CnB binding pocket and wherein said method comprises the steps of:

a) selecting a subset of CnA/CnB amino acid structure coordinates according to Figure 1, which are provided on a computer, to define all or part of said CnA/CnB binding pocket;

b) utilizing said structure coordinates defining all or part of said CnA/CnB binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

c) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the CnA/CnB binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

d) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with all or

part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

56. (new) A method of using a computer for selecting at least one of a plurality of chemical entities based on its ability to associate with all or part of a molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 124, 150, 151, 156, 159, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 310, 311, 312, 313, 314, 317, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;
wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining all or part of said CnA/CnB binding pocket and wherein said method comprises the steps of:

a) selecting a subset of CnA/CnB amino acid structure coordinates according to Figure 1, which are provided on a computer, to define all or part of said CnA/CnB binding pocket;

b) utilizing said structure coordinates defining all or part of said CnA/CnB binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

c) docking said chemical entity with all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of all or part of the CnA/CnB binding pocket or the chemical entity, wherein said docking utilizes energy minimization;

d) analyzing the results of said docking to quantify the association between said chemical entity and all or part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

e) optionally repeating steps a) through d) with another of said plurality of chemical entities; and

f) selecting at least one of said plurality of chemical entities that associates with all or

part of the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.